Nuclear Lattice EFT: Status & Perspectives

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CONTENTS

• Nuclear lattice EFT - what and why?
• Chiral EFT on a lattice
• Algorithmic developments
  – the shuttle algorithm
  – the pinhole algorithm
  – the pinhole trace algorithm
• Essentials of nuclear binding
• Ab initio nuclear thermodynamics
• Summary & outlook
Nuclear lattice EFT: what and why?
• Theoretical methods:
  – Lattice QCD: $A = 0, 1, 2, \ldots$
  – NCSM, Faddeev-Yakubovsky, GFMC, ... : $A = 3 - 10$
  – coupled cluster, ...: $A = 10 - 100$
  – density functional theory, ...: $A \geq 10(0)$

• Chiral EFT:
  – provides accurate 2N, 3N and 4N forces
  – successfully applied in light nuclei with $A = 2, 3, 4$

  Epelbaum, Hammer, UGM, Rev. Mod. Phys. 81 (2009) 1773

  – combine with simulations to get to larger $A$

⇒ Nuclear Lattice Effective Field Theory

• Nuclear structure:
  ★ 3-nucleon forces
  ★ limits of stability
  ★ alpha-clustering

• Nuclear scattering: processes relevant for nuclear astrophysics
  ★ alpha-particle scattering: $^4\text{He} + ^4\text{He} \rightarrow ^4\text{He} + ^4\text{He}$
  ★ triple-alpha reaction: $^4\text{He} + ^4\text{He} + ^4\text{He} \rightarrow ^{12}\text{C} + \gamma$
  ★ alpha-capture on carbon: $^4\text{He} + ^{12}\text{C} \rightarrow ^{16}\text{O} + \gamma$

MANY–BODY APPROACHES

- nuclear physics = notoriously difficult problem: strongly interacting fermions

- define *ab initio*: combine the precise and well-founded forces from *chiral EFT* with a many-body approach

- two different approaches followed in the literature:

  ★ combine chiral NN(N) forces with standard many-body techniques

  Dean, Duguet, Hagen, Navratil, Nogga, Papenbrock, Schwenk, Soma . . .

  → successful, but problems with cluster states (SM, NCSM,...)

  ★ combine chiral forces and lattice simulations methods

  → this new method is called *Nuclear Lattice Effective Field Theory (NLEFT)*

  Borasoy, Elhatisari, Epelbaum, Krebs, Lee, Lähde, UGM, Rupak, . . .

  → rest of the talk
# COMPARISON to LATTICE QCD

<table>
<thead>
<tr>
<th>LQCD (quarks &amp; gluons)</th>
<th>NLEFT (nucleons &amp; pions)</th>
</tr>
</thead>
<tbody>
<tr>
<td>relativistic fermions</td>
<td>non-relativistic fermions</td>
</tr>
<tr>
<td>renormalizable th’y</td>
<td>EFT</td>
</tr>
<tr>
<td>continuum limit</td>
<td>no continuum limit</td>
</tr>
<tr>
<td>(un)physical masses</td>
<td>physical masses</td>
</tr>
<tr>
<td>Coulomb - difficult</td>
<td>Coulomb - easy</td>
</tr>
<tr>
<td>high T/small (\rho)</td>
<td>small T/nuclear densities</td>
</tr>
<tr>
<td>sign problem severe</td>
<td>sign problem moderate</td>
</tr>
</tbody>
</table>

- similar methods:
  - hybrid MC, parallel computing, . . .
  - only treated briefly (shuttle algorithm)

- what I want to discuss within the time limitations:
  - how to put the chiral EFT on a lattice
  - the pinhole algorithm / center-of-mass in AFQMC
  - the pinhole trace algorithm
  - going to larger \(A\), increasing the precision
  - \textit{ab initio} nuclear thermodynamics

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Chiral EFT on a lattice

T. Lähde & UGM

*Nuclear Lattice Effective Field Theory - An Introduction*

Springer Lecture Notes in Physics 957 (2019) 1 - 396
new method to tackle the nuclear many-body problem

discretize space-time \( V = L_s \times L_s \times L_s \times L_t \): nucleons are point-like particles on the sites

discretized chiral potential w/ pion exchanges and contact interactions + Coulomb

\[ \rightarrow \text{see Epelbaum, Hammer, UGM, Rev. Mod. Phys. 81 (2009) 1773} \]

typical lattice parameters

\[ p_{\text{max}} = \frac{\pi}{a} \simeq 314 \text{ MeV [UV cutoff]} \]

\[ \sim 2 \text{ fm} \]

strong suppression of sign oscillations due to approximate Wigner SU(4) symmetry


physics independent of the lattice spacing for \( a = 1 \ldots 2 \text{ fm} \)

\[ \text{Alarcon, Du, Klein, Lähde, Lee, Li, Lu, Luu, UGM, EPJA 53 (2017) 83; Klein, Elhatisari, Lähde, Lee, UGM, EPJA 54 (2018) 121} \]
LATTICE NOTATION

- nucleon annihilation ops: \( a_{0,0} \equiv a_{↑,p}, \ a_{1,0} \equiv a_{↓,p}, \ a_{0,1} \equiv a_{↑,n}, \ a_{1,1} \equiv a_{↓,n} \)

  \( \rightarrow \) labeling spin and isospin

- spatial & temporal lattice spacing: \( a, a_t \rightarrow \alpha_t \equiv a_t / a \)

- lattice size: \( L \equiv N a, \ L_t \equiv N_t a_t \)

- lattice momenta: \( \vec{k} = (k_1, k_2, k_3) \equiv \left( \frac{2\pi}{N} \hat{k}_1, \frac{2\pi}{N} \hat{k}_2, \frac{2\pi}{N} \hat{k}_3 \right) \)

  \( \rightarrow \) in the first Brillouin zone: \( |k_i| < \pi \) and \( 0 \leq |\hat{k}_i| < N/2 \)

- any derivative operator requires improvement, as the simplest representation in terms of two neighboring points is afflicted by the largest discretization errors

  \[ k_l \equiv \sum_{j=1}^{\nu+1} (-1)^{j+1} \theta_{\nu,j} \sin(jk_l) + \mathcal{O}(a^{2\nu+2}) \]

  \[ \frac{1}{2} k^2_l \equiv \sum_{j=0}^{\nu+1} (-1)^j \omega_{\nu,j} \cos(jk_l) + \mathcal{O}(a^{2\nu+2}) \]

  \( \rightarrow \) no improvement (\( \nu = 0 \)): \( \theta_{0,1} = 1, \ \omega_{0,0} = 1, \ \omega_{0,1} = 1 \)
LATTICE NOTATION continued

• Order $a^2$ improvement ($\nu = 1$): $\theta_{1,1} = \frac{4}{3}, \theta_{1,2} = \frac{1}{6}, \omega_{1,0} = \frac{5}{4}, \omega_{1,1} = \frac{4}{3}, \omega_{1,2} = \frac{1}{12}$

• Order $a^4$ improvement ($\nu = 2$): $\theta_{2,1} = \frac{3}{2}, \theta_{2,2} = \frac{3}{10}, \theta_{2,3} = \frac{1}{30}$
  $\omega_{2,0} = \frac{49}{36}, \omega_{2,1} = \frac{3}{2}, \omega_{2,2} = \frac{3}{20}, \omega_{2,3} = \frac{1}{90}$

$\nabla_{l,(\nu)} f(\vec{n}) \equiv \frac{1}{2} \sum_{j=1}^{\nu+1} (-1)^j \theta_{\nu,j} [f(\vec{n} + j\hat{e}_l) - f(\vec{n} - j\hat{e}_l)]$

$\tilde{\nabla}^2_{l,(\nu)} f(\vec{n}) \equiv -\sum_{j=0}^{\nu+1} (-1)^j \omega_{\nu,j} [f(\vec{n} + j\hat{e}_l) + f(\vec{n} - j\hat{e}_l)]$

has two zeros in per Brillouin zone $\rightarrow$ beneficial feature for tuning NLO coefficients

$\tilde{\omega}^{(\nu)}(\vec{p}) \equiv \frac{1}{\tilde{m}_N} \sum_{j=0}^{\nu+1} \sum_{l=1}^{3} (-1)^j \omega_{\nu,j} \cos(jp_l)$

$\tilde{m}_N \equiv m_N a$

TRANSFER MATRIX METHOD

• Correlation–function for A nucleons: 
  \[Z_A(\tau) = \langle \Psi_A | \exp(-\tau H) | \Psi_A \rangle\]
  with \(\Psi_A\) a Slater determinant for A free nucleons
  [or a more sophisticated (correlated) initial/final state]

• Transient energy
  \[E_A(\tau) = -\frac{d}{d\tau} \ln Z_A(\tau)\]
  \(\rightarrow\) ground state:  
  \[E_A^0 = \lim_{\tau \to \infty} E_A(\tau)\]

• Exp. value of any normal–ordered operator \(\mathcal{O}\)
  \[Z_A^\mathcal{O} = \langle \Psi_A | \exp(-\tau H/2) \mathcal{O} \exp(-\tau H/2) | \Psi_A \rangle\]
  \[\lim_{\tau \to \infty} \frac{Z_A^\mathcal{O}(\tau)}{Z_A(\tau)} = \langle \Psi_A | \mathcal{O} | \Psi_A \rangle\]
⇒ all possible configurations are sampled
⇒ preparation of all possible initial/final states
⇒ clustering emerges naturally
Represent interactions by auxiliary fields:

\[
\exp \left[ -\frac{C}{2} (N^\dagger N)^2 \right] = \sqrt{\frac{1}{2\pi}} \int ds \exp \left[ -\frac{s^2}{2} + \sqrt{C} \, s \,(N^\dagger N) \right]
\]

optimally suited for parallel computing!

COMPUTATIONAL EQUIPMENT

- Past = JUQUEEN (BlueGene/Q)
- Present = JUWELS (modular system) + SUMMIT + ...
Algorithmic developments


pinhole trace algorithm: Lu et al., arXiv:1912.05105, subm. for publication
THE SHUTTLE ALGORITHM

- Auxiliary fields $s(n_t, \vec{n})$ are updated on one time slice only

- Proceed to the next time slice, update, ... , turn around at the end of the time series

→ very efficient for small temporal lattice spacings, $a_t = 0.001$ MeV$^{-1}$

→ high acceptance rate, typically $\sim 50\%$

→ more efficient than HMC

→ about 10 times more configurations per hour generated

→ further acceleration by GPUs

AFQMC calculations involve states that are superpositions of many different center-of-mass (com) positions

\[
Z_A(\tau) = \langle \Psi_A(\tau) | \Psi_A(\tau) \rangle
\]

\[
|\Psi_A(\tau)\rangle = \exp(-H\tau / 2) |\Psi_A\rangle
\]

but: translational invariance requires summation over all transitions

\[
Z_A(\tau) = \sum_{i_{\text{com}}, j_{\text{com}}} \langle \Psi_A(\tau, i_{\text{com}}) | \Psi_A(\tau, j_{\text{com}}) \rangle, \quad \text{com} = \text{mod}((i_{\text{com}} - j_{\text{com}}), L)
\]

\[
i_{\text{com}} (j_{\text{com}}) = \text{position of the center-of-mass in the final (initial) state}
\]

→ density distributions of nucleons can not be computed directly, only moments

→ need to overcome this deficiency
PINHOLE ALGORITHM

- Solution to the CM-problem:
  track the individual nucleons using the *pinhole algorithm*

- Insert a screen with pinholes with spin & isospin labels that allows nucleons with corresponding spin & isospin to pass = insertion of the A-body density op.:

\[ \rho_{i_1,j_1,\ldots,i_A,j_A}(n_1, \ldots, n_A) = : \rho_{i_1,j_1}(n_1) \cdots \rho_{i_A,j_A}(n_A) : \]

- MC sampling of the amplitude:

\[ A_{i_1,j_1,\ldots,i_A,j_A}(n_1, \ldots, n_A, L_t) = \langle \Psi_A(\tau/2)|\rho_{i_1,j_1,\ldots,i_A,j_A}(n_1, \ldots, n_A)|\Psi_A(\tau/2) \rangle \]

- Allows to measure proton and neutron distributions

- Resolution scale \( \sim a/A \) as cm position \( r_{cm} \) is an integer \( n_{cm} \) times \( a/A \)

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PROTON and NEUTRON DENSITIES in CARBON

- first NLEFT calculation of the charge density in $^{12}$C [proton size accounted for]
- asymptotic properties of the distributions from the volume dependence of N-body bound states
- open symbols: neutron / closed symbols: proton

$\Rightarrow$ independent of projection time $\rightarrow$ ground state
$\Rightarrow$ small error bars $\rightarrow$ sign problem under control


FORM FACTORS

- Fit charge distributions by a Wood-Saxon shape
  - get the form factor from the Fourier-transform (FT)
  - uncertainties from a direct FT of the lattice data

⇒ detailed structure studies become possible
PINHOLE TRACE ALGORITHM (PTA)

- The pinhole states span the whole $A$-body Hilbert space

- The canonical partition function can be expressed using pinholes:

$$Z_A = \text{Tr}_A \left[ \exp(-\beta H) \right], \quad \beta = 1/T$$

$$= \sum_{n_1, \cdots, n_A} \int \mathcal{D}s \mathcal{D}\pi \langle n_1, \cdots, n_A | \exp[-\beta H(s, \pi)] | n_1, \cdots, n_A \rangle$$

- allows to study: liquid-gas phase transition → this talk
  
  thermodynamics of finite nuclei
  
  thermal dissociation of hot nuclei
  
  cluster yields of dissociating nuclei

Essentials of Nuclear Binding

B. N. Lu, N. Li, S. Elhatisari, D. Lee, E. Epelbaum, UGM,
TOWARDS HEAVY NUCLEI in NLEFT

- Two step procedure:

1) Further improve the LO action
   - minimize the sign oscillations
   - minimize the higher-body forces
   - gain an understanding of the essentials of nuclear binding

2) Work out the corrections to N3LO
   - first on the level of the NN interaction
   - second for the spectra of nuclei
   - third for nuclear reactions (nuclear astrophysics)
ESSENTIAL ELEMENTS for NUCLEAR BINDING I


• **Step 1**: construct a highly improved LO action, free of any sign problem

• Highly SU(4) symmetric LO action without pions, local and non-local smearing:

\[
H_{SU(4)} = H_{\text{free}} + \frac{1}{2!} C_2 \sum_n \tilde{\rho}(n)^2 + \frac{1}{3!} C_3 \sum_n \tilde{\rho}(n)^3
\]

\[
\tilde{\rho}(n) = \sum_i \tilde{a}_i^\dagger(n) \tilde{a}_i(n) + s_L \sum_{n'-n=1} \sum_i \tilde{a}_i^\dagger(n') \tilde{a}_i(n')
\]

\[
\tilde{a}_i(n) = a_i(n) + s_{NL} \sum_{|n'-n|=1} a_i(n')
\]

• **Only four** parameters!

\[ C_2 \text{ and } C_3 = \text{strength of the leading two- and three-body interactions} \]

\[ s_L \text{ and } s_{NL} = \text{strength of the local and the non-local interaction} \]
ESSENTIAL ELEMENTS for NUCLEAR BINDING II

• Fixing the parameters:
  ★ interaction strength $C_2$ and range $s_L$ from the average S-wave scattering lengths and effective ranges (requires SU(4) breaking later)
  ★ interaction strength $C_3$ from the $^3$H binding energy
  ★ interaction range $s_{NL}$ can not be determined in light nuclei
  $\hookrightarrow$ calculate the volume- and surface energy of mid-mass nuclei $16 \leq A \leq 40$

• compare w/ existing calculations:

$\hookrightarrow S_{NL} = 0.5$

FRLDM: Möller et al., Atom Data Nucl. Data Tabl. 59 (1995) 184
mean field: Bender et al., Rev. Mod. Phys. 75 (2003) 121
ENERGIES for SELECTED NUCLEI

- Calculated binding energies for 3N & alpha-type nuclei:

<table>
<thead>
<tr>
<th></th>
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<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>$^3$H</td>
<td>8.48(2)*</td>
<td>0.0</td>
<td>1.00</td>
</tr>
<tr>
<td>$^3$He</td>
<td>7.75(2)</td>
<td>0.73(1)</td>
<td>1.00</td>
</tr>
<tr>
<td>$^4$He</td>
<td>28.89(1)</td>
<td>0.80(1)</td>
<td>1.02</td>
</tr>
<tr>
<td>$^{16}$O</td>
<td>121.9(3)</td>
<td>13.9(1)</td>
<td>0.96</td>
</tr>
<tr>
<td>$^{20}$Ne</td>
<td>161.6(1)</td>
<td>20.2(1)</td>
<td>1.01</td>
</tr>
<tr>
<td>$^{24}$Mg</td>
<td>193.5(17)</td>
<td>28.0(2)</td>
<td>0.98</td>
</tr>
<tr>
<td>$^{28}$Si</td>
<td>235.8(17)</td>
<td>37.1(4)</td>
<td>1.00</td>
</tr>
<tr>
<td>$^{40}$Ca</td>
<td>346.8(8)</td>
<td>71.7(6)</td>
<td>1.01</td>
</tr>
</tbody>
</table>

[* = input]

- selected nuclei: amazingly precise, largest deviation about 4% in $^{16}$O
- even-even isotopic chains come out amazingly precise, general trends reproduced
  ↬ on the proton-rich side better than on the neutron-rich one → spin-dep. effects
- but remember: this is only leading order!
RADII for SELECTED NUCLEI

- Calculated charge radii for 3N & alpha-type nuclei:

<table>
<thead>
<tr>
<th></th>
<th>$R_{ch}$</th>
<th>Exp.</th>
<th>$R_{ch}$/Exp.</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^3\text{H}$</td>
<td>1.90(1)</td>
<td>1.76</td>
<td>1.08</td>
</tr>
<tr>
<td>$^3\text{He}$</td>
<td>1.99(1)</td>
<td>1.97</td>
<td>1.01</td>
</tr>
<tr>
<td>$^4\text{He}$</td>
<td>1.72(3)</td>
<td>1.68</td>
<td>1.02</td>
</tr>
<tr>
<td>$^{16}\text{O}$</td>
<td>2.74(1)</td>
<td>2.70</td>
<td>1.01</td>
</tr>
<tr>
<td>$^{20}\text{Ne}$</td>
<td>2.95(1)</td>
<td>3.01</td>
<td>0.98</td>
</tr>
<tr>
<td>$^{24}\text{Mg}$</td>
<td>3.13(2)</td>
<td>3.06</td>
<td>1.02</td>
</tr>
<tr>
<td>$^{28}\text{Si}$</td>
<td>3.26(1)</td>
<td>3.12</td>
<td>1.04</td>
</tr>
<tr>
<td>$^{40}\text{Ca}$</td>
<td>3.42(3)</td>
<td>3.48</td>
<td>0.98</td>
</tr>
</tbody>
</table>

- Radii quite well described
  $\rightarrow$ overcomes earlier problems (see PRL 109 (2012) 252501, 112 (2014) 102501)

- Charge distributions for $^{16}\text{O}$ and $^{40}\text{Ca}$

- Also a fair description of the charge distributions at LO!
NEUTRON MATTER

- 14 to 66 neutrons in $L = 5, 6, 7 \rightarrow \rho = 0.02 - 0.15 \text{ fm}^{-3}$

- exact SU(4)
  \( \leftrightarrow \) deviations at low densities

- SU(4) breaking term \( \rightarrow a_{nn} \)
  \( \leftrightarrow \) good overall description

GOING to HIGHER ORDERS

- **Step 2:** Work out NN phase shifts to N3LO
  - calculate nuclear properties based on NN forces only \( \checkmark \)
  - add three-nucleon forces (in the works)

- Starting Hamiltonian:

\[
H_{2N} = H_{\text{free}} + H_{SU(4)}(C_3 = 0) + H_{OPE}
\]

  - consistent with the power counting (3NFs appear at N2LO)
  - OPE induces some sign problem (but manageable)

- NN forces to N3LO worked out for 4 latt. spacings \( a = 0, 99, 1.32, 1.64, 1.98 \) fm
  with local and non-local smearing and restoration of Galilean invariance breaking
  - used as input for nuclear structure calculations

NN INTERACTION at N3LO

• np phase shifts including uncertainties for $a = 1.64$ fm (cf. Nijmegen PWA)
NUCLEI at N3LO

- Binding energies of nuclei for $a = 1.64 \text{ fm}$

\[ \begin{align*}
  &\text{Experiment} \\
  &E_{\text{LO}} \\
  &E_{\text{N3LO}}
\end{align*} \]

$\rightarrow$ excellent starting point for precision studies

Ab Initio Nuclear Thermodynamics

B. N. Lu, N. Li, S. Elhatisari, D. Lee, J. Drut, T. Lähde, E. Epelbaum, UGM, [arXiv:1912.05105], submitted for publication
Phase diagram of strongly interacting matter

- Superfluid
- Liquid-vapor
- Vapor
- Gas
- Supercritical fluid
- Quark-gluon plasma

Fig. courtesy B.-N. Lu
NEW PARADIGM for NUCLEAR THERMODYNAMICS

• The PTA allows for simulations with fixed neutron & proton numbers at non-zero $T$ 
  $\rightarrow$ thousands to millions times faster than existing codes using the 
  grand-canonical ensemble ($t_{\text{CPU}} \sim VN^2$ vs. $t_{\text{CPU}} \sim V^3N^2$)

• Only a mild sign problem $\rightarrow$ pinholes are dynamically driven to form pairs

• Typical simulation parameters:
  
  up to $N = 144$ nucleons in volumes $L^3 = 4^3, 5^3, 6^3$
  $\rightarrow$ densities from $0.008 \text{ fm}^{-3}$ ... $0.20 \text{ fm}^{-3}$
  
  $a = 1.32 \text{ fm} \rightarrow \Lambda = \pi/a = 470 \text{ MeV} \ , \ a_t \simeq 0.1 \text{ fm}$
  
  consider $T = 10 \ldots 20 \text{ MeV}$

• use twisted bc’s, average over twist angles $\rightarrow$ acceleration to the td limit

• very favorable scaling for generating config’s: $\Delta t \sim N^2L^3$
CHEMICAL POTENTIAL

- Calculated from the free energy:  \[ \mu = \frac{F(N + 1) - F(N - 1)}{2} \]
EQUATION of STATE

- Calculated by integrating: \(dP = \rho \, d\mu\)
- Critical point: \(T_c = 15.8(1.6)\, \text{MeV},\ P_c = 0.26(3)\, \text{MeV/fm}^3,\ \rho_c = 0.089(18)\, \text{fm}^{-3}\)
VAPOR-LIQUID PHASE TRANSITION

- Vapor-liquid phase transition in a finite volume $V$ & $T < T_c$
- the most probable configuration for different nucleon number $A$
- the free energy
- chemical potential $\mu = \partial F/\partial A$
SUMMARY & OUTLOOK

- Nuclear lattice simulations: a new quantum many-body approach
  → based on the successful continuum nuclear chiral EFT
  → a number of highly visible results already obtained

- Algorithmic developments
  → shuttle algorithm speeds up the simulations considerably
  → pinhole algorithm allows to fix the center-of-mass: charge distributions etc
  → pinhole trace algorithm: thermodynamics with fixed nucleon number

- Towards heavier nuclei & higher precision
  → highly improved LO action based on SU(4) → nuclei & neutron matter
  → NN interaction at N3LO, first results for nuclei at N3LO

- Ab initio nuclear thermodynamics
  → partition function via the pinhole trace algorithm
  → first promising results for the phase diagram of nuclear matter at finite temperature
  → prediction of the vapor-liquid phase transition within reasonable accuracy